

# Zitterbewegung in monolayer silicene in a magnetic field

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## Abstract

We study the Zitterbewegung in monolayer silicene under a perpendicular magnetic field. Using an effective Hamiltonian, we have investigated the autocorrelation function and the density currents in this material. Moreover, we have analyzed other types of periodicities of the system (classical and revival times). Finally, the above results are compared with their counterparts in two other monolayer materials subject to a magnetic field: graphene and MoS<sub>2</sub>

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*Introduction.* Silicene is a monolayer of Silicon atoms theoretically predicted some years ago [1, 2] and experimentally observed in 2010 [3, 4, 5, 6, 7]. It has a honeycomb structure similar to that of graphene and its low-energy electronic properties can also be described by an effective Dirac-type Hamiltonian for each of the two inequivalent corners of the Brillouin zone [8, 9, 10, 11, 12, 13]. Silicene has a band gap of 1.55 meV due to a relative large spin-orbit coupling which can be experimentally controlled by applying a perpendicular electric field. Interesting physical properties have been investigated in this material, as a quantum valley Hall effect or topological phase transitions.

On the other hand, Zitterbewegung (ZB) appears in Dirac particles as a rapid trembling motion around their otherwise rectilinear average trajectory, as a consequence of the interference between eigenstates with positive and negative eigenvalues. Recently, there have been many theoretical studies of ZB, not only in relativistic systems but also in condensed matter systems (see the review by Rusin and Zawadski [14] and references therein). ZB has not been experimentally observed yet due to its large frequency and small amplitude, but it has been simulated experimentally by means of trapped ions (adjusting some parameters of the Dirac equation) by Gerritsma et al. [15]. ZB has been studied in different types of monolayer and bilayer graphene devices [14, 16, 17, 18, 19, 20, 21, 22, 24, 25].

In this Letter, we shall describe ZB in silicene in a perpendicular magnetic field. Additionally, we shall show that there is a regeneration of the ZB ampli-

tude for appropriate wave packets's initial conditions. Next, we shall introduce the effective Hamiltonian for silicene and then study the ZB and revivals. Finally, we shall compare the results with two other monolayer materials, namely, graphene and MoS<sub>2</sub>.

*Model Hamiltonian.* Let us consider a monolayer silicene in a perpendicular magnetic field  $B$  with an effective Hamiltonian given by [8]

$$H_s^\tau = v_F(\sigma_x p_x - \tau \sigma_y p_y) - \tau s \Delta \sigma_z, \quad (1)$$

where  $\tau = \pm 1$  corresponds respectively to the inequivalent corners  $\mathbf{K}$  and  $\mathbf{K}'$  of the Brillouin zone,  $\mathbf{p}$  stands for the momentum,  $\boldsymbol{\sigma}$  is the Pauli matrices vector,  $v_F = 5 \times 10^5$  m/s is the Fermi velocity of the Dirac fermions, with up and down spin values being represented by  $s = \pm 1$ , and  $\Delta$  is the band gap induced by intrinsic spin-orbit interaction, which provides a mass to the Dirac fermions. Using the Landau gauge,  $\mathbf{A} = (0, Bx, 0)$ , the eigenvalues can be written as [8]

$$E_{sn\gamma}^\tau = \gamma \sqrt{n\epsilon^2 + \Delta^2}, \quad (2)$$

with  $\gamma = \pm 1$  accounting for the valence and conduction bands and  $\epsilon = \sqrt{2}\hbar v_F/l_B \approx 0.1794\sqrt{B(T)}$  eV. The corresponding eigenfunctions at the  $\mathbf{K}$  point are given by

$$\Phi_{sn\gamma}(\mathbf{r}) = e^{ik_y y} \begin{pmatrix} \alpha_{\gamma,n} \langle x|n-1\rangle \\ \beta_n \langle x|n\rangle \end{pmatrix}, n \geq 1, \quad (3)$$

$$\begin{pmatrix} |0\rangle \\ 0 \end{pmatrix}, n = 0. \quad (4)$$

Here,  $\alpha_{\gamma,n} = \Delta + \gamma\sqrt{\Delta^2 + n\epsilon^2}$ ,  $\beta_n = -i\sqrt{n}\epsilon$  and with normalization given by  $N_{\gamma,n} = \sqrt{|\alpha_{\gamma,n}|^2 + |\beta_n|^2}$ . The eigenfunctions at the  $\mathbf{K}'$  ( $\tau = -1$ ) point are obtained by exchanging electron and hole components in the above case. We shall take  $\Delta = 4$  meV. The eigenvalues and eigenvectors do not depend on the values of  $s$  within this level of approximation, so we do not take into account the spin of the electron in this study

*Wave packet temporal evolution.* The evolution of a wave packet for a time independent Hamiltonian is given by (in units such that  $\hbar = 1$ )

$$\Psi(t) = \sum_{n=0}^{\infty} a_n u_n e^{-iE_n t} \quad (5)$$

$u_n$  and  $E_n$  being the eigenfunctions and eigenvalues, respectively, and  $a_n = \langle u_n, \Psi \rangle$ . If we consider an initial wave packet localized around the energy  $E_{n_0}$  of the spectrum  $E_n$ , then a Taylor expansion of the energy can be written as

$$E_n \approx E_{n_0} + E'_{n_0}(n - n_0) + \frac{E''_{n_0}}{2}(n - n_0)^2 + \dots \quad (6)$$

and, consequently,

$$\begin{aligned} & \exp(-iE_n t) = \\ & \exp\left(-i\left[E_{n_0} + E'_{n_0}(n - n_0) + \frac{E''_{n_0}}{2}(n - n_0)^2 + \dots\right]t\right) \\ & \exp\left(-iE_{n_0}t - \frac{2\pi i(n - n_0)t}{T_{Cl}} - \frac{2\pi i(n - n_0)^2t}{T_R} + \dots\right), \end{aligned} \quad (7)$$

where each term defines an important characteristic time scale. In particular, the so-called revival time  $T_R \equiv 4\pi/|E''_{n_0}|$  is the time the wave packet needs to return to a shape that is approximately the same as the initial one in the temporal evolution, and the classical period,  $T_{Cl} \equiv 2\pi/|E'_{n_0}|$ , is the time over which the wave packet follows the expected classical trajectory (see [22] and references therein for more details).

Furthermore, we shall study ZB in the wave packet evolution. To this purpose, we have elected as the initial state a superposition of two wave packets with both positive and negative energy levels, which we denote respectively by  $E_n^{(+)}$  and  $E_n^{(-)}$ , and with associated eigenfunctions  $u_n^{(+)}$  and  $u_n^{(-)}$ . To be concrete,

$$\psi = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-) \quad (8)$$

with

$$\begin{aligned} \psi_+ &= \sum_{n=0}^{\infty} c_n^{(+1)} \Phi_{sn1}(x, y), \\ \psi_- &= \sum_{n=0}^{\infty} c_n^{(-1)} \Phi_{sn-1}(x, y). \end{aligned} \quad (9)$$

Under these conditions, ZB will appear as an additional periodicity in the wave packet evolution given by  $T_{ZB} = \pi/E_{n_0}$  [22]. Lastly, we mention that the choice of our initial wave packet is one used in many theoretical works, but for experimental purposes it should be taken into account that it has recently been described how to create more realistic wave packets by illuminating Carbon nanotubes with short laser pulses [23].

*Results.* First, we shall consider the ZB in the wave packet evolution in monolayer silicene. Both packets (see Eq. 9) are centered around the same value of  $n_0 = 11$ , and with coefficients Gaussianly distributed as

$$c_n^{(\pm 1)} = c_n = \left(\frac{1}{\pi\sigma^{1/2}}\right)^{1/2} \exp\left(-\frac{(n - n_0)^2}{2\sigma}\right). \quad (10)$$

Other parameter values are  $B = 1\text{T}$ ,  $\sigma = 3$  and  $s = 1$ . The subsequent time evolution of this initial state is then monitored by the computation of the au-

to correlation function,  $A(t)$ , customarily defined as

$$A(t) = \int dx dy \Psi^*(x, y, 0) \Psi(x, y, t). \quad (11)$$

Notice that a value of  $|A(t)|^2$  close to unity implies that the initial and the time-evolved wave packets must have a significant overlap. We shall make use of this quantity to identify the several types of periodicity in the temporal development of the wave packet, namely, ZB, classical motion and revivals. These can be calculated analytically using Eq. (2) and read

$$T_{\text{ZB}} = \frac{\pi}{\gamma \sqrt{\Delta^2 + \epsilon^2 n}}, \quad T_{\text{Cl}} = \frac{4\pi \sqrt{\Delta^2 + \epsilon^2 n}}{\epsilon^2 \gamma},$$

$$T_{\text{R}} = \frac{16\pi(\Delta^2 + \epsilon^2 n)^{3/2}}{\epsilon^4 \gamma}.$$

Figure 1 shows the time dependence of  $|A(t)|^2$  at the three different time scales. The top panel represents the ZB of electrons with  $T_{\text{ZB}} \simeq 0.47$  fs; in the middle panel the first classical periods of motion can be appreciated, with  $T_{\text{Cl}} \simeq 0.15$  ps; the bottom panel displays the long time revival behavior with  $T_{\text{R}} \simeq 3.3$  ps along with the several fractional revivals occurring at intervening times. The main fractional revivals are indicated by vertical, dotted lines, where  $T_{\text{R}}$  is calculated from its analytical expression  $T_{\text{R}} = 4\pi/|E''_{n0}|$ .

Additionally, we have also studied the time dependence of electronic currents and how they are affected by the three above-mentioned types of oscillatory motion. In particular, since the electron velocity operators are given by  $v_j = i[H, r_j]/ = v_F \sigma_j$ , with  $j = x, y$ , it is straightforward to obtain  $j_x(t) = 0$  and

$$j_y(t) = 2ev_F \sum_{n=0}^{\infty} c_n c_{n-1} \xi_n 2 \cos(E_n t) \cos(E_{n-1} t). \quad (12)$$

with  $\xi_n = [(\alpha_{+,n}/N_{+,n}) + (\alpha_{-,n}/N_{-,n})]/\beta_{n-1}$ .

Figure 2 shows the influence of ZB on the current in the femtosecond scale (top panel); ZB oscillations can be clearly seen superimposed on the classical ones at medium times (middle panel); revivals of the electric current can be recognized at  $T_{\text{R}}$  and fractional revivals at, for instance,  $T_{\text{R}}/2$  and  $3T_{\text{R}}/4$ , in the picosecond scale (bottom panel).

Next, we extend the previous study to MoS<sub>2</sub> and graphene. The Hamiltonian for the former is identical to that of monolayer silicene except for its smaller gap  $\Delta = 0.775$  eV, Fermi velocity  $v_F = 85000$  m/s, and consequently  $\epsilon \simeq 30.510^{-3} \sqrt{B}$ . In the case of graphene, within the tight binding approximation and near the vicinity of the  $\mathbf{K}$  point, one of the two inequivalent corners of the Brillouin zone, the Hamiltonian reads as in Eq. (1) but now with  $\Delta = 0$  and the Fermi velocity  $10^6$  m/s.

In Figure 3 results are compared for silicene, MoS<sub>2</sub> and graphene. The top panel shows that the ZB time is almost insensitive to the intensity of the magnetic field for MoS<sub>2</sub> (red, long dashed line), whilst it rapidly decays for silicene

(brown, short dashed line) and graphene (blue, solid line). The classical periods are compared in the central panel, where it can be appreciated that MoS<sub>2</sub> behaves differently in that its classical time is almost two orders of magnitude higher than those of silicene and graphene for any  $B$ . The same trend repeats in the bottom panel, showing that the revival times of silicene and graphene are similar, but that of MoS<sub>2</sub> is approximately two orders of magnitude higher at large  $B$  and four or more orders of magnitude higher at low  $B$ . As  $B$  approaches zero, ZB times for MoS<sub>2</sub>, silicene and graphene converge to finite values that are of the same order of magnitude. The revival and classical times diverge when  $B$  approaches zero in the three cases.

*Summary.* We have studied the current oscillations due to ZB in silicene under a magnetic field, by considering wave packets with a Gaussian population of both positive and negative energy levels. Additionally, the ZB time is compared with other periodicities that arise when the wave packets are peaked around a sufficiently large quantum number, namely the classical period and the revival times. As in a previous study [22], we find  $T_{\text{ZB}} < T_{\text{Cl}} < T_{\text{R}}$ , with  $T_{\text{ZB}}$  in the femtosecond scale and  $T_{\text{Cl}}, T_{\text{R}}$  in the picosecond scale for a moderate intensity of the magnetic field,  $B = 1$  T. A comparison with MoS<sub>2</sub> and graphene reveals that despite these three materials share a similar hexagonal monolayer structure the classical and revival time scales of MoS<sub>2</sub> are largely different from those of silicene and graphene. Interestingly, also MoS<sub>2</sub>'s ZB times differ drastically from silicene and graphene, showing that  $T_{\text{ZB}}$  for MoS<sub>2</sub> is almost insensitive to the strength of the magnetic field. We conclude by mentioning that there is a great interest in the experimental observation of ZB and, in this regard, we point out a recent relevant proposal to observe this phenomenon by using the techniques of quantum optics [26].

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## References

- [1] K. Takeda, K. Shiraishi, Phys. Rev. B 50 (1994) 14916.
- [2] G. G. Guzman-Verri, L. Lew Yan, Phys. Rev. B 76 (2007) 075131.
- [3] P. Vogt et al., Phys. Rev. Lett. 108 (2012) 155501.
- [4] B. Augray, A. Kara, S. B. Vizzini, H. Oughaldou, C. LéAndri, B. Ealet, G. Le Lay, App. Phys. Lett. 96 (2010) 183102.
- [5] B. Lalmi, H. Oughaddou, H. Enriquez, A. Kara, S. B. Vizzini, B. N. Ealet, B. Augray, App. Phys. Letters 97 (2010) 223109.
- [6] A. Feurence, R. Friedlein, T. Ozaki, H. Kawai, Y. Wang, Y. Y. Takamura, Phys. Rev. Lett. 108 (2012) 245501.
- [7] P. E. Padova et al., App. Phys. Lett. 96 (2010) 261905.

- [8] M. Tahir, U. Schwingenschlögl, Sci. Rep. 3 (2013) 1075.
- [9] M. Ezawa, New J. Phys. 14 (2012) 033003.
- [10] M. Ezawa, J. Phys. Soc. Jpn. 81 (2012) 064705.
- [11] N. D. Drummond, V. Zólyomi, V. I. Fal'ko, Phys. Rev. B 85 (2012) 075423.
- [12] M. Ezawa, Phys. Rev. B 86 (2012) 161407 (R).
- [13] M. Ezawa, Phys. Lett. A 378 (2014) 1180.
- [14] W. Zawadzki, T. M. Rusin, J. Phys. Condens. Matter 23 (2011) 143201.
- [15] R. Gerritsma, G. Kirchmair, F. Zahringer, E. Solano, R. Blatt, C. F. Roos, Nature (London) 463 (2010) 68.
- [16] T. M. Rusin, W. Zawadzki, Phys. Rev. B 76 (2007) 195439; 78 (2008) 125419; 80 (2009) 045416.
- [17] J. Cserti and G. Dávid, Phys. Rev. B 74 (2006) 172305, Phys. Rev. B 82 (2010) 201405(R); G. Dávid and J. Cserti, Phys. Rev. B 81 (2010) 121417(R).
- [18] M. I. Katsnelson, Europ. Phys. J. B 51 (2006) 157.
- [19] G. M. Maksimova, V. Y. Demikhovskii, E. V. Frolova, Phys. Rev. B 78 (2008) 235321.
- [20] J. C. Martínez, M. B. A. Jalil, S. G. Tan, Appl. Phys. Lett. 97 (2010) 062111.
- [21] J. Schliemann, New J. Phys. 10 (2008) 034024.
- [22] E. Romera, F. de los Santos, Phys. Rev. B 80 (2009) 165416.
- [23] T. M. Rusin, W. Zawadzki, J. Phys. Cond. Matter 26 (2014) 215301.
- [24] Y. X. Wang, Z. Yang, S. J. Xiong, Eur. Phys. Lett. 89 (2010) 17007.
- [25] T. García, N. A. Cordero, E. Romera, Phys. Rev. B 89 (2014) 075416.
- [26] T. Rusin and W. Zawadzki arXiv: 1404.6187 (2014).

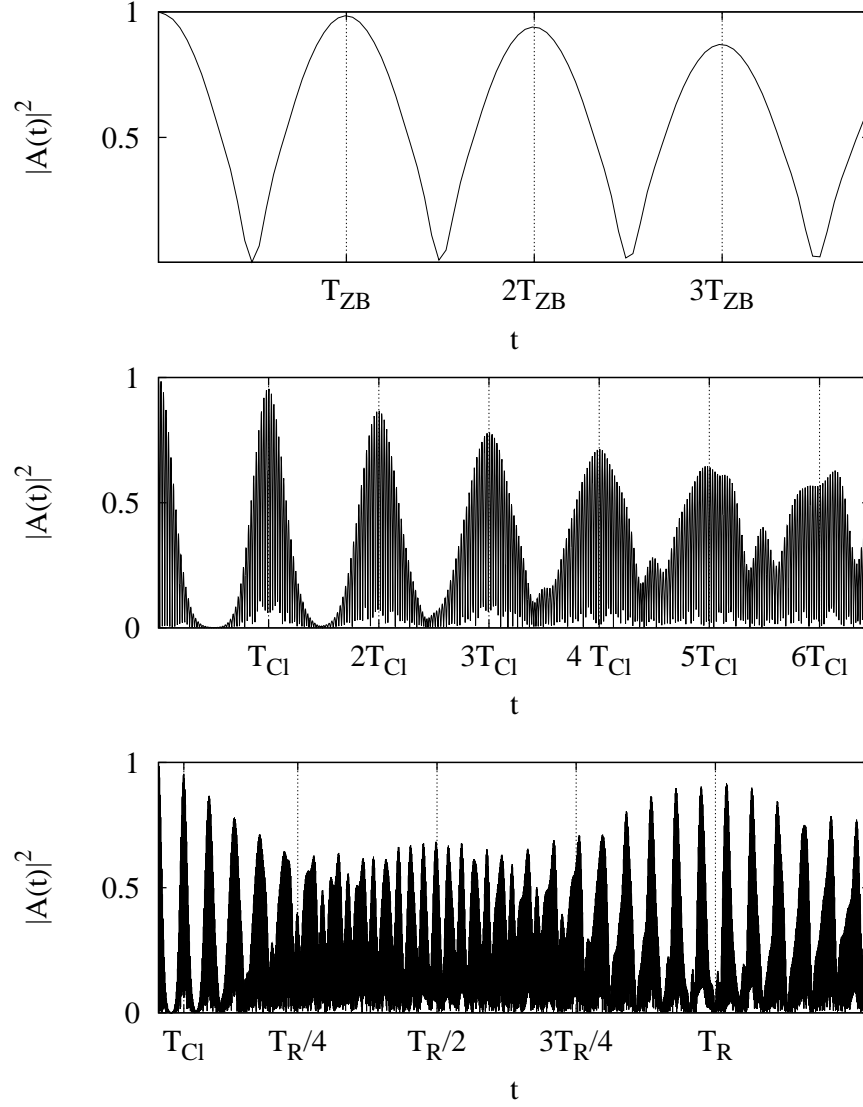


Figure 1: Time dependence of the autocorrelation function  $|A(t)|^2$  in silicene for  $B = 1$  T,  $n_0 = 11$ ,  $\sigma = 3$ , a band gap  $\Delta = 4$  meV, and  $s = 1$ . (top panel) ZB of electrons with  $T_{\text{ZB}} \simeq 3.47$  fs (central panel) First classical periods of motion with  $T_{\text{Cl}} \simeq 0.15$  ps. (bottom panel) Long-time dependence with  $T_{\text{R}} \simeq 3.3$  ps. The Zitterbewegung, classical periods and the main fractional revivals are indicated by vertical dotted lines.

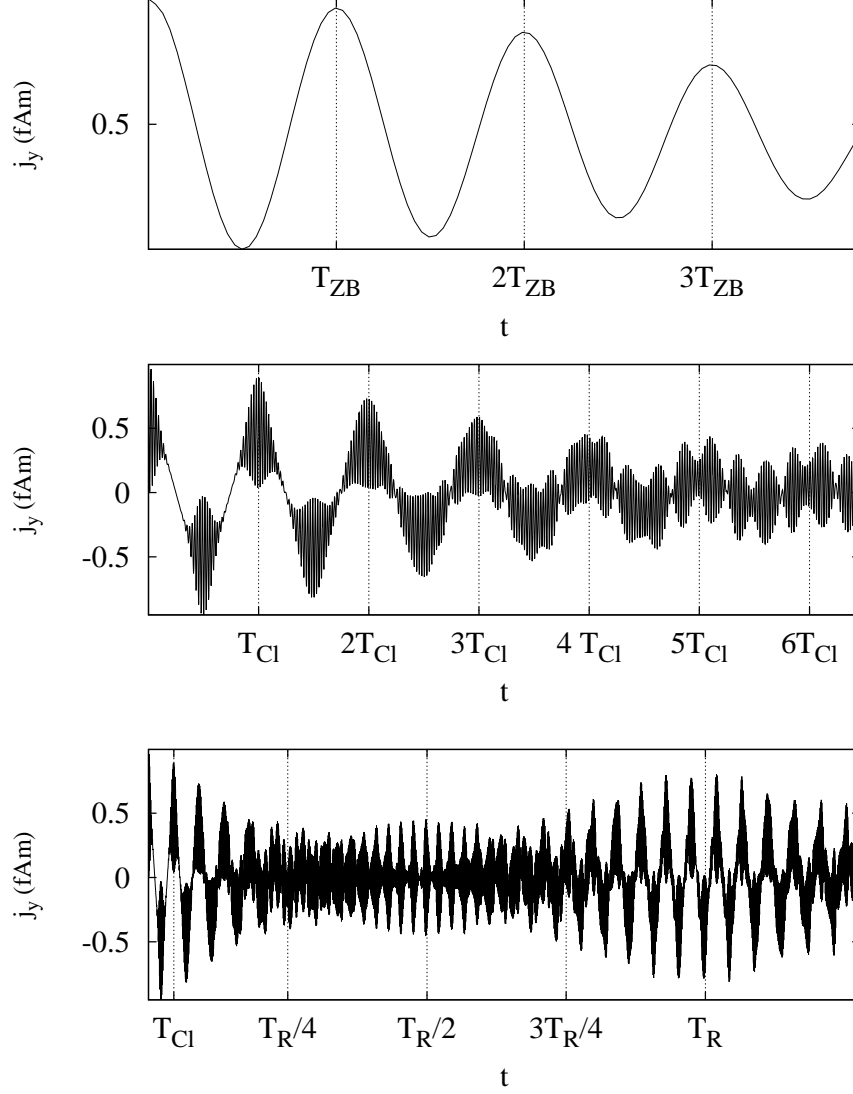


Figure 2: Time dependence of electric currents  $j_y$  in silicene for  $B = 1$  T,  $n_0 = 11$ ,  $\sigma = 3$ , a band gap  $\Delta = 4$  meV and  $s = 1$ . (Top panel) ZB of electrons with  $T_{ZB} \simeq 3.47$  fs. (Middle panel) First classical periods of motion with  $T_{Cl} \simeq 0.15$  ps. (Bottom panel) Long-time dependence with  $T_R \simeq 3.3$  ps. The Zitterbewegung, classical periods and the main fractional revivals are indicated by vertical dotted lines.



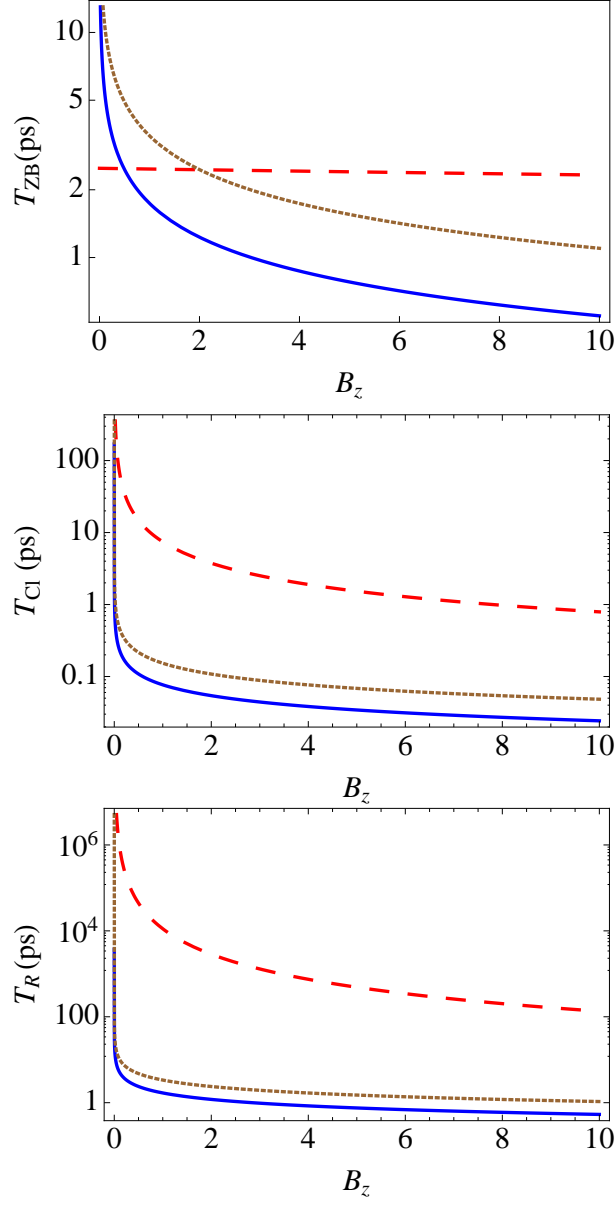


Figure 3: ZB (Top panel), classical (middle panel), and revival times (bottom panel) for silicene (brown, short dashed line), MoS<sub>2</sub> (red, long dashed line), and graphene (blue, solid line).